Optimization of Product Grade Transition by Model Predictive Control

L. Dobos, S. Németh, J. Abonyi

Department of Process Engineering, Pannon University

Veszprém, H-8200 Egyetem út 10
POB 158

ABSTRACT

The production of synthetic polymers represents an important part of chemical industry. In these processes it is common that the same process is used for the production of different kind of products (various molecular weights, compositions, etc.). Therefore, beside the optimization of the operating conditions related to the production of different products, it is also important to minimize the time of the grade transition reducing the amount of off-specification products.

This optimization can be considered as an optimal control problem. Among the wide range of tools and algorithms can be used to solve optimal control problems this paper studies the applicability of model predictive control (MPC) solutions. In the chemical industry the influence of MPC is increasing, they are very successful in wide range of industrial applications. This became possible because more and more algorithms are available for the implementation of model predictive controllers. MPC requires a proper model for the prediction of the effect of the current control signal to allow its optimization. It is important to note that the nonlinear behavior of the process mainly appears during grade transitions than at steady state operation. This phenomenon would require the utilization of nonlinear models in the controller. However, the application of nonlinear first-principles models is restricted due to the formulation of these models requires the identification of large amount of kinetic parameters, which can be very time-consuming and costly.

In these situations the applications of data-driven models could be more beneficial. Hence this paper MPC solution for the optimization of grade transitions based on input/output data driven models is studied.

The free radical polymerization reaction of methyl-metacrylate is considered using azobisisobutironitil (AIBN) as initiator, and toulene as solved. The aim of the process is producing different kind of grades, and the number-average molecular weight was for identify the right state of process, and it can be influenced by the inlet initiator flow rate. The proposed controller is compared to the wide-spread applied PID controllers and the control performances results are qualified the ISE (integral Square of Error) criteria.

Using the impulse response and the step response models of the reactor, Dynamic Matrix Controller as MPC has been designed. The results show that the performance of the model predictive controller is better than the performance of PID controller, which is also proved by the ISE criteria.

Keywords: MPC, predictive control, polymerization, impulse response

INTRODUCTION

The production of the synthetic polymers represents an important part of chemical industry. In this industrial segment it is usual that one reactor is used for producing different kind of products (various molecular weights, compositions, etc.).

During transitions between products, off-spec products are produced. This product is generally worth less than the on-spec material; therefore it is of interest to minimize its production. The on-spec material can be produced under varying circumstances and at varying operating points, which are more or less economically sound, motivating optimization of the production during production stages.

In these processes a large number of different grades are produced, and the transition times between the productions may be relatively long and costly in comparison with the total amount produced. The optimization of complex operating processes generally begins with a detailed investigation of the process and its control system. It is important to know, how databased information can support the optimization of product transition strategies. The optimization of product grade transition is a typical example for complex optimization in process industry [6].

It is common to define an objective function, for example minimize the grade transition time, this way reducing off-specification products. The nonlinear behavior mainly appears during grade transitions, so handling these transitions are a complex and difficult problem to solve, so-called optimization strategies are time-consuming to define.

The control of polymerization reactors can be difficult and complex problem, for example due to the nonlinear dynamic behavior, the multiplicities of steady states, parametric sensitivity. One kind of problem is the large amount of kinetic parameters, which are essential for creating a first principle model, but obtaining these parameters can be very time-consuming from the literature, laboratories, pilot-plants, and sometimes it is possible that the kinetic mechanism should not be available which can also make difficulties while making the first principle model. So it is useful to find those methods, where these pieces of information are not

necessary, so model can be crated from input-output data, by identifying the model parameters, and an appropriate controller can be developed for the process from these data.
Unfortunately it is very difficult the find the right tuning parameters in the whole operation range because of the nonlinearity of the process, and identified models from input output data are mostly linear.
Since the process trajectory within a processing stage depends on the process trajectory of the preceding stage, the rigorous approach is to treat the production optimization problem as a whole, including phases of transition as well as phases of production. This can be considered as a large-size real-time optimization (RTO) or dynamic real-time optimization (DRTO) problem [2], in which optimal set points or trajectories are calculated in order to minimize economic objectives subject to constraints. Several algorithms have been published to effectively solve this production optimization problem using dynamic optimization. These advanced algorithms can be formulated as a so-called multistage dynamic optimization problem, where the production time is split up into several processing stages. Most of these tools require accurate model of the process, which is not always available.
Treating this kind of optimization problems is the main target for us, and this paper would be an introduction to the optimization methods. In the industry the influence of model predictive control is increasing [3], they are very successful in wide range of industrial applications. This is true because more and more algorithm are available for planning model predictive controllers. It can be useful to compare the widespread applied PID controllers, and the increasingly applied model predictive controllers. For this study we choose a PI controller to compare with a dynamic matrix controller, and we qualified the performance with ISE (integral Square of Error) criteria.
Paper is organized as follows: the description of the polymerization process, define the purposes, introduce the theoretical basis of the solution and present the results.

THE CASE STUDY
INVESTIGATION OF A POLYMERIZATION PROCESS

Process description

The reactor what have been studied is a SISO (single input-single output) process, a CSTR where a free radical polymerization reaction of methyl-metacrylate is considered using azobisisobutironitil (AIBN) as initiator, and toulene as solved. The aim of the process is to produce different kinds of product grades. The number-average molecular weight is used for qualifying the product and process state, and it can be influenced by the inlet initiator flow rate. When this assumption is considered, and the effect of the temperature is neglected, the multi input-multi output model could be reduced to a SISO process. Because of the isothermal assumption a four-state model can be obtained. [4]

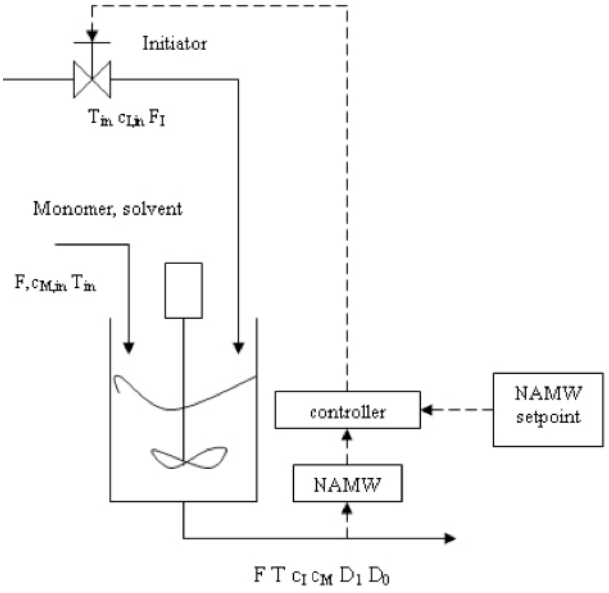

Fig. 1 The configuration of SISO process

$$\frac{dC_m}{dt} = -(k_p + k_{fm})C_m P_0 + \frac{F(C_{m,in} - C_m)}{V} \quad (1.)$$

$$\frac{dC_I}{dt} = -k_I C_I + \frac{F_I C_{I,in} - FC_I}{V} \quad (2.)$$

$$\frac{dD_0}{dt} = (0.5k_{Tc} + k_{Td})P_0^{\ 2} + k_{f_m} C_m P_0 - \frac{FD_0}{V} \quad (3.)$$

$$\frac{dD_1}{dt} = M_m(k_p + k_{fm})P_0 C_m - \frac{FD_1}{V} \quad (4.)$$

$$y = \frac{D_1}{D_0} \quad (5.)$$

where:

$$P_0 = \left[\frac{2f * k_I C_I}{k_{Td} + k_{Tc}}\right]^{0.5} \quad (6.)$$

where:
C_m - concentration of the monomer in the reactor
$C_{m,in}$ - monomer concentration in feed
C_I - initiator concentration in the reactor
$C_{I,in}$ - initiator concentration in feed
D0 - zero order moment of the chain length distribution
D_1 - first order moment of the chain length distribution
k_p, k_{fm}, k_I, k_{Tc}, k_{Td} - kinetic parameters

D_0 is the zero order moment of the chain length distribution of the inactive polymer chain, which represents the lenght of inacitve chains. D_1 is the first order moment of inactive polymer chains which means the distribution of molecular weight of inactive chains. And *y* represents the number average molecular weight,

which can not be measured, but it is calculated, as can be seen in the 5. equation.

The nominal values of the process model, and the value of the kinetic parameters are given in Table (1).

k_{Tc}=	1.3281×10^{10}	m3/(kmol*h)
k_{Td}=	1.0930×10^{11}	m3/(kmol*h)
k_I=	1.0224×10^{-1}	1/h
k_p=	2.4952×10^{6}	m3/(kmol*h)
k_{fm}=	2.4522×10^{3}	m3/(kmol*h)
f*=	0.58	
F=	1.0	m3/h
V=	0.1	m3
$C_{I,in}$=	8.0	kmol/m3
M_m=	100.12	kg/kmol
$C_{m,in}$=	6.0	kmol/m3

Table (1) – kinetic parameters and nominal values of the process model

Problem description

The task is producing three different kind of grades, called A, B, C.

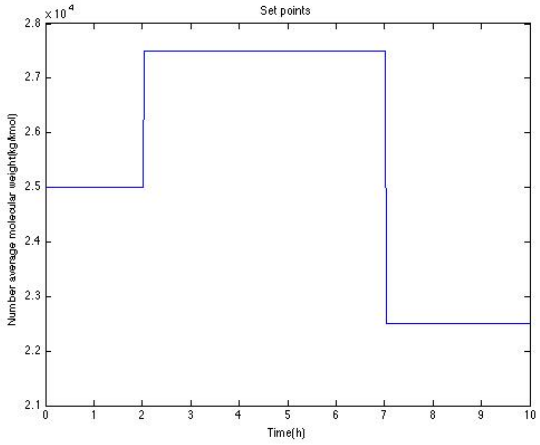

Fig. 2 set points of the grade transitions

'A' grade is produced in the first two hours with the number average molecular weight (NAMW) 25000 kg/kmol. After 'B' grade would be produced during the next five hours with the NAMW 27500 kg/kmol. The 'C' grade is the terminating grade in this study which is produced in the last three hours with the NAWM 22500 kg/kmol.

The main goal is to minimize the amount of the off-grade product, so reduce the grade transition time as much as possible to show that there are reserved, untapped possibilities in the the process, and the model predictive controllers can have better performance than original PI controllers.

MPC BASED FORMULATION OF OPTIMAL GRADE TRANSITION

Model Predictive Controllers– theoretical basis

MPC is a model based control algorithm where the models are used to predict the behavior of dependent variables (i.e. outputs) of a dynamical system with respect to changes in the process independent variables (i.e. inputs). In chemical processes, independent variables are most often setpoints of regulatory controllers that govern valve movement (e.g. valve positioners with or without flow, temperature or pressure controller cascades), while dependent variables are most often constraints in the process (e.g. product purity, equipment safe operating limits). The MPC uses the models and current plant measurements to calculate future moves in the independent variables that will result in operation that honors all independent and dependent variable constraints. The MPC then sends this set of independent variable moves to the corresponding regulatory controller setpoints to be implemented in the process. With the help of the Figure (3) the essence of the model predictive controlling is easily understandable:

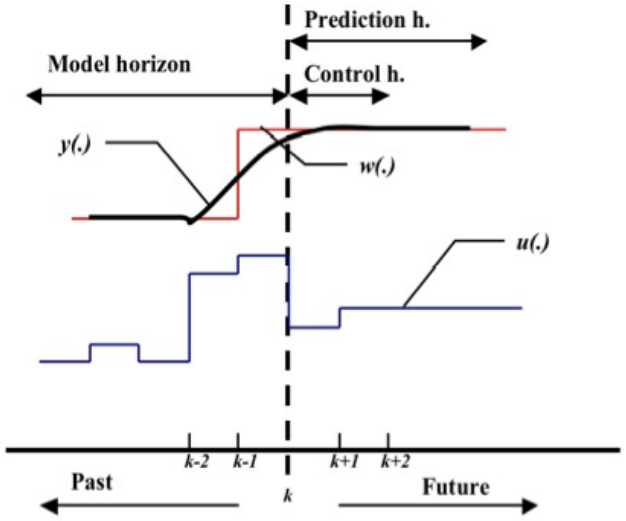

Fig. 3 The essence of model predictive controlling

Formulating the aim of the method, an objective function is the result, which is:

$$\min_{\Delta u(k+j)} \sum_{j=H_{p1}}^{H_{p1}} (w(k+j)-y(k+j))^2 + \lambda \sum_{j=1}^{H_c} \Delta u^2(k+j-1) \qquad (7.)$$

where $w(k+j)$ means the set point value, $y(k+j)$ means the predicted dependent value in the $(k+j)th$ discrete time moment, Δu means the incremention of the control signal, λ is an weight parameter.

The black box model – Impulse response model

The identification of the dynamic part of a block-oriented model is a challenging task. In practice, the identification of the parameters of the IRM may be troublesome due to the large number of them [7].
In this case the identification parameters can be obtained easily using φ variable which means:

$$\varphi(i) = y(i) - y(i-1) \tag{8.}$$

where y(i) is the output of the process in the ith moment. With the help of φ the parameters of the discrete impulse response model (IRM) can be calculated easily:

$$g_i = \frac{\varphi(i)}{\sum_{i=1}^{N} \varphi(i)} \tag{9.}$$

where Δt denotes the sampling time, *i* the *i*th discrete time-step, and *N is* the model horizon. This results in a more parsimonious IRM model description, where the variance of the identification problem is decreased by the decrease of the number of the parameters to be estimated.

The model based predictive controller

The convolution model can be easily applied in model predictive control scheme. The control algorithm is based on the natural division of the system response into *free* and *forced* response terms [1]:

$$y_m(k+t) = y_{forced}(k+t) + y_{free}(k+t) \tag{10.}$$

where the forced output, $y_{forced}(k+t)$, depends only on the future inputs,

$$y_{forced}(k+t) = K\sum_{i=1}^{t} s_i \Delta u(k+t-i) \tag{11.}$$

where $\{s_i\}$ are the gain independent step response coefficients defined by $s_i = \sum_{j=1}^{i} g_j$; and $\Delta u(k+t-i)$ denotes the change on the control variable: $\Delta u(k+t-i) = u(k+t-i) - u(k+t-i-1)$.
As the previous equation suggests, the forced response is calculated by using a linear model, because the steady state gain, *K*, is calculated at the *k*th time step, and is assumed to be constant during the prediction. In control engineering practice such one step linearization is commonly used for simplifying the highly computational-demanding optimisation task. The proposed method differs from these approaches in the calculation of the *free response* of the system that represents the effect of the previous control signals that can interpreted as the future response of the process assuming that the process input is constant during the prediction horizon, H_p. Hence, convolution model is used to generate this *free response*, $y_{free}(k+i) = Q_i + y_s$, where the Q_i coefficients are [5]:

$$Q_i = \sum_{t=1}^{i} \sum_{j=t+1}^{N} g_j \Delta u(k+t-j),$$

$$i = 1,2,..,H_p . \tag{12.}$$

The future incremental control actions, $w = \left[w(k+1), \mathrm{K}\ , w(k+H_p)\right]^T$, are obtained by minimising the following cost function:

$$\min_{\Delta \mathbf{u}} = \left(w - \left(K\mathbf{S}\Delta\mathbf{u} + \mathbf{y}_{free}\right)\right)^2 + \lambda \Delta \mathbf{u}^2 \tag{13.}$$

where w is the set point vector $w = \left[w(k+1), \mathrm{K}\ , w(k+H_p)\right]^T$ denotes the future set-point values, $\mathbf{y}_{free} = \left[y_{free}(k+1), \mathrm{K}\ , y_{free}(k+H_p)\right]^T$ the predicted free-response, and **S** is the gain independent dynamic matrix:

$$\mathbf{S} = \begin{bmatrix} s_1 & 0 & 0 & \mathrm{L} & 0 \\ s_2 & s_1 & 0 & & 0 \\ s_3 & s_2 & s_1 & \mathrm{O} & 0 \\ \mathrm{M} & \mathrm{M} & \mathrm{M} & & \mathrm{M} \\ s_{H_c} & s_{H_c-1} & s_{H_c-2} & & s_1 \\ \mathrm{M} & \mathrm{M} & \mathrm{M} & & \mathrm{M} \\ s_{H_p} & s_{H_p-1} & s_{H_p-2} & \mathrm{L} & s_{H_p-H_c+1} \end{bmatrix}_{H_p \times H_c} \tag{14.}$$

The move suppression coefficient, λ, employs a punishment for the variation of the manipulated variable. For nonlinear processes this constant can be gain-scaled by expressing it as a product of a scaled move-suppression coefficient, γ, and the square of the process gain, $\lambda = \gamma \cdot K^2$ [8].
If the process constraints are not taken into account, the previous minimisation problem can be solved effectively by least-squares method,

$$\Delta u = \frac{1}{K} \cdot (S^T \cdot S + \gamma \cdot I)^{-1} \cdot S^T \cdot e \tag{15.}$$

where **e** is the vector of the estimated errors $\mathbf{e} = \mathbf{r} - \mathbf{y}_{free}$, and **I** is a unity matrix.
The controller has three parameters. These are the prediction horizon, H_p, the control horizon, H_c, and the gain independent move suppression coefficient, γ. The prediction horizon should roughly be equal to the 60% of the open loop settling time to ensure controller stability. When the process in nonlinear, the open-loop settling time is changing with the operating point. According to this effect, the prediction horizon can be adapted during the operation. A simpler solution is setting the prediction horizon equal to the 60% of maximum of the settling time. In the application study of this paper we consider the linear model of the process, and we consider the move-suppression coefficient, $\lambda = 4.8529 * 10^{10}$. The value of the move suppression coefficient was obtained with a parameter sensitivity examination, which can be seen later

in Figure (6), because the move suppression coefficient depends on the length of the control horizon. [8].

$$\lambda = \gamma \cdot K^2 \qquad (16.)$$

$$\gamma = 0 \quad \text{if } C=1 \qquad (17.)$$

$$\gamma = \frac{C}{500}\left(\frac{3.5 \cdot \tau_p}{T} + 2 - \frac{(C-1)}{2}\right) \quad \text{if } C>1 \qquad (18.)$$

Where:
C – length of the control horizon
T – sample time
τ_p – time constant of the first order and dead time model of the process

MODEL PREDICTIVE CONTROL OF A SISO POLYMERIZATION PROCESS

Model Identification

For this study we generated input-output data with the white-box model, using sample time Ts=0.03h. We identificated our black-box model by these data-sets. Our black box model is the impulse response model and the step response model, the integral of IRM.
Because of the nonlinearity of the white box model, we have chosen a steady state point and we identified our black box model around this point. After identification the model was validated, because of the control of its' reliability.

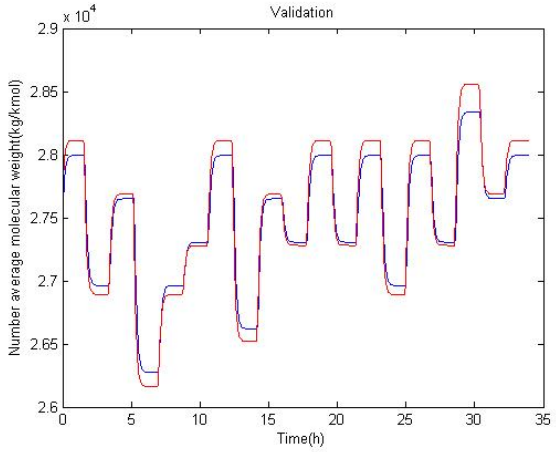

Fig. 4 Validation of black box model

In this picture the red line means the input output point generated by the white box model, the blue line means the calulated point with the black box model. This figure shows that the identification succeded, because the black box model correlates the process well.

Results

The tuning parameters were selected to obtain satisfactory set-point tracking and disturbance rejection. Setpoint changes mean grade change.We have studied a PI controller and a model predictive contoller, DMC. The control signal is between the range u=[0.0046, 0.05] m^3/h in both cases. The PI controller was implemented to the white box model and, the parameters of it is obtained the following way: a first order plus dead time model was identificated and due to this model the tuning parameters of PI controller could be obtained with ITAE method, and it can provide a good result, as it can be seen in the following figure:

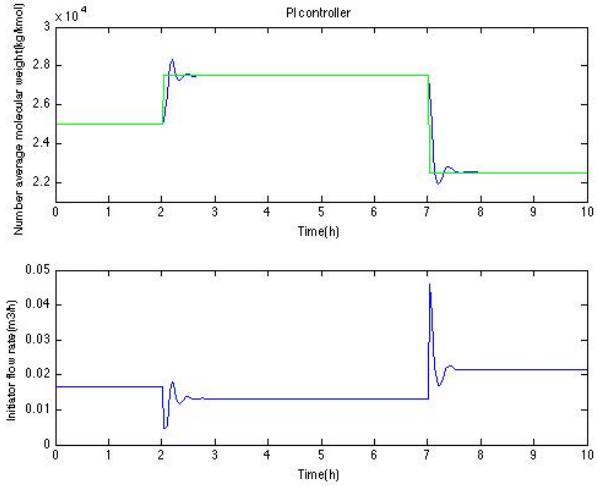

Fig. 5 simulation with PI controller

The PI parameters: K=-6.78*10^{-6} TI=0.225 h, which can ensure a good kind of controlling. So the new set point (from 25000 kg/kmol to 27500 kg/kmol) is obtained in 1 hour, with a overshoot with approximately ¼ decay ratio, and an other set point change in 7th hour, and the new set point is obtained in an hours.(green line is the set point signal, blue is the measured signal(NAWM) in both cases). So the length of the grade transition time can be seen a little bit long, so finding a method is neccessary to reduce the grade transition time, or finding a control algorithm which can provide producing less off-grade product.
It is necessary to qualify the two controllers and to realize it a criteria was needed, and due to this it was possible to compare them with each other. The ISE (Integral Square of Error) criteria was chosen to satisfy this demand. Examining the figures the advantage of any controller is very difficult to state. The error of the PI controller was 3.8418*10^7, and it would be rewarding to compare to the following performance of the DMC controller.
The model predictive controller provides very different kind of controlling due to little overshoot. The set point is the same like in the case of PI controller, because of the comperableness.
The tuning parameters of DMC, is the lenght of the prediction horizon, control horizon, and the value of the γ parameter, and it is also important to define the lenght of model horizon. The value of the move suppression coefficient depends on the lenght of the control horizon and the parameters of the first order and dead time model [8]. The model horizon is *N*=30, which was obtained by using the impulse response model (IRM) of process. The most effective value of tuning parameters can be reached with analysis their effects on the qualifying parameter, the ISE value. This effect can be seen in the Figure(6).

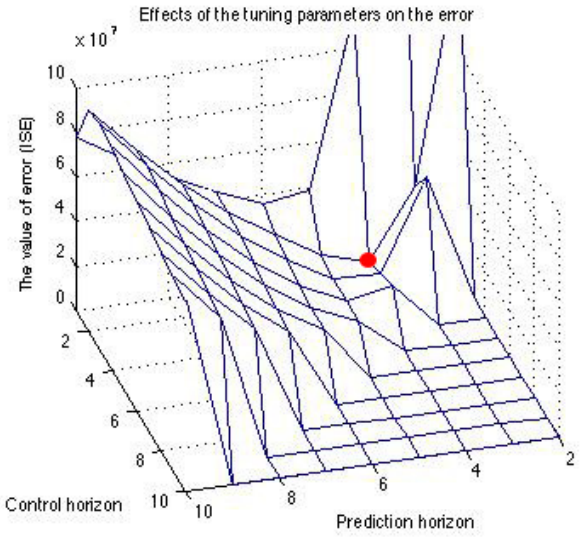

Fig.6 Effect of tuning parameters on Integral Square of Error

In this figure the 0 values of the error is not reachable, because it is not permitted to have larger value of the control horizon than the predicitve horizon, so disqualifying these values a minimum value of the error can be seen (red point), so the parameters of this minimum place can be the ideal tuning parameters of the DMC controller.

The prediction horizon is selected to be p=4 because, as the Figure 6 shows, increasing the prediction horizon the quality of controlling is getting worse. The control horizon is selected to be c=2, because when the length of the control horizon converges the value of the prediction horizon the controller becomes more aggressive, and it causes increasing error.

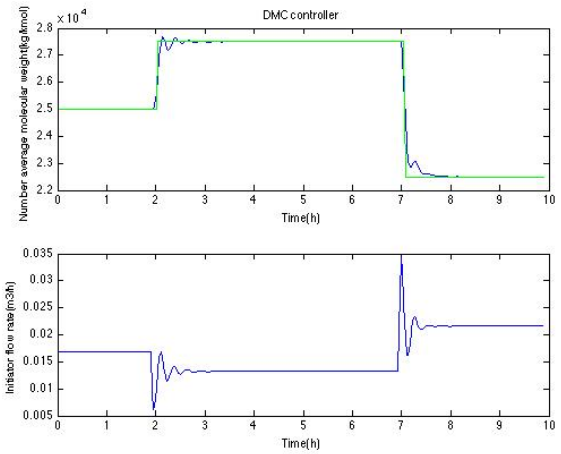

Fig. 7 simulation with DMC controller.

Obtaining the tuning parameters of the model predicitive controller can be considered as an optimization problem where the objective function is to minimize the ISE value. It would be mixed integer optimization problem and it is the next task to solve it.

The behavior of DMC controller is definitely different to the PI controller, but the DMC can be a little bit faster than the PI controller and has irrelevant overshoot. Comparing the DMC to the PI controller, the DMC can afford $1.3412*10^7$ error. So the advantage of model predictive can be stated. Tuning these two controllers more agressively would result additional oscillations, and lenghten the time it takes for them to keep the number average of molecular weight in in accurate value, so a compromise is needed to be made in tuning the controllers for servo-mode.

CONCLUSION

In the chemical industry the importance of the polymerization processes is increasing. To develop these processes the length of the grade transitions are needed to reduce, because this way it becomes possible to avoid to produce off-grade products. To reach this demand a MPC algorithm was used to handle the grade transitions. In this work a PI and a MPC controller were compared each other. First we use the first-principle model of a polymerization process, and using this the black box model was identified. Using the impulse response and the step response model of the reactor, the DMC could be build for this reactor. It is seen that the performance of the model predictive controller is better, than the performance of PI algorithm. It is also proved by the ISE criteria. Generally, it is very important to find the best fitting controller algorithm to realize the objective function. In a lot of cases the advantage of MPC algorithms fits better to these objective function, but they have a huge disadvantage: in most cases it is necessary to use linear model approaches which are very sensitive for the identified parameters, and in nonlinear systems these parameters can change different kind of methods are available. The non-linear model predictive controllers can handle this problem, or adaptive algorithms are able to solve them. Regarding to the the increasing spread of MPC controllers, because of the rising industrial demand, it would be useful to develop the nonlinear model predictive controllers, because of the hope of better performance of the whole operating range.

Acknowledgements

The authors would like to acknowledge the support of the Cooperative Research Center (VIKKK) (project 2003-I), and founding from the Hungarian Research Found (OTKA T 049534 and T037600). Janos Abonyi is grateful for the financial support of the Janos Bolyai Research Fellowship of the Hungarian Academy of Science.

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Correspondig author:
János Abonyi
University of Pannonia, Department of Process Engineering
H-8200 Veszprém, P.O.Box 158.
Pannon Egyetem, Folyamatmérnöki Intézeti Tanszék
8200 Veszprém, Pf 158.
e-mail:abonyij@fmt.uni-pannon.hu